

# MESO - Mesoscale Atmospheric Transport and Diffusion Code

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## ABSTRACT

MESO is a Lagrangian particle transport and diffusion code that provides high-fidelity downwind hazard predictions for a wide range of chemical and biological agents and munitions. Developed by ITT Industries through sponsorship with the Department of Defense, MESO incorporates state-of-the-art meteorology with full chemical and biological agent capabilities. MESO can ingest and use three-dimensional time-dependant wind fields, and spatially varying surface characteristics to produce solutions in complex terrain. Current MESO efforts include the development of concentration variance computations, verification and validation, continued atmospheric boundary layer improvements, and enhanced user friendliness.

**Introduction** - MESO is a high-fidelity code that is currently under development for the Naval Surface Warfare Center to simulate atmospheric transport and dispersion anywhere from the ground up to and above the tropopause. MESO uses tracer particles undergoing random-walk excursions to simulate the movement of contaminate gases and particles in turbulent flow. The tracer techniques are substantially faster than standard particle-in-a-cell or finite-difference methods, and a typical high-altitude release can be simulated on a PC in about five minutes. The technique is immune to both numerical instabilities and artificial diffusion, and requires no grid. Vertical resolutions on the order of only 5 to 20 meters can be rapidly modeled even for high-altitude releases and long-range transport. Since the code is accurate to second order in time, numerical accuracy is primarily limited by the number of particles selected by the user. Because the code models advection by direct movement of the tracer particles with the wind field, the code is capable of accurately modeling both high wind shear and large downwind transport distances, without the usual inaccuracies common to both Eulerian or Gaussian puff codes. To illustrate the tracer nature of the code, tracer positions are plotted in Figure 1 shown 100 s after their release in both stable and unstable conditions. The pronounced difference in the cloud shapes is a result of the much higher daytime mixing rates, which not only disperse the tracers more rapidly but also modifies the wind profile. MESO can operate on a single wind profile or can ingest a full 3D wind field, such as from a forecast code, and allows differing surface characteristics and meteorology from cell to cell. If only a single wind speed is known at a reference height, MESO computes a profile using the surface roughness and stability.

**Stochastic Tracer Techniques** – For continuous releases (plumes) the code uses the random walk techniques developed by Diehl et al. (1982) for vertical dispersion and standard Langevin techniques (van Dop et al., 1985) for horizontal dispersion. In the limit of an infinite number of tracers, the random walk technique can be shown to be a gradient transfer process. In contrast, with the Langevin technique tracers are moved in a manner consistent with the known properties of the turbulence. For vertical dispersion the random walk method is only accurate to first order in daytime conditions after the boundary layer has fully developed. However, it is numerically fast compared to other stochastic techniques and in stable conditions is much faster than Langevin techniques.

For instantaneous releases (clouds), dispersion must be handled in a different manner than for plume dispersion. Large eddies transport the cloud, but do not disperse it. Only eddies whose size is on the order of the cloud size or smaller are effective in dispersing the cloud. Thus, as the cloud grows in size, larger and larger eddies come into play until the cloud exceeds the size of the largest turbulence length scales. The methodology used by MESO to expand a cluster of particles, i.e. cloud, is based on the scale-dependent mixing theory proposed by Smith and Hay (1961). A short discussion of this technique is a part of many textbooks on dispersion, for example, Nieuwstadt and Van Dop (1982) and Pasquill and Smith (1983). The growth rate is a function of the ratio of the cloud size to the Eulerian length scale. For horizontal growth, the cloud is divided into layers each with its own growth rate. For vertical dispersion, the cloud is taken as a whole.

Tracer dispersion for clouds is computed using the random-walk technique of Diehl et al. (1982). However, the diffusivity used in the calculation is based on the scale-dependent mixing theory of Smith and Hays. The prescription for the diffusivity is based on the Lagrangian length scale of the turbulence and the standard deviation

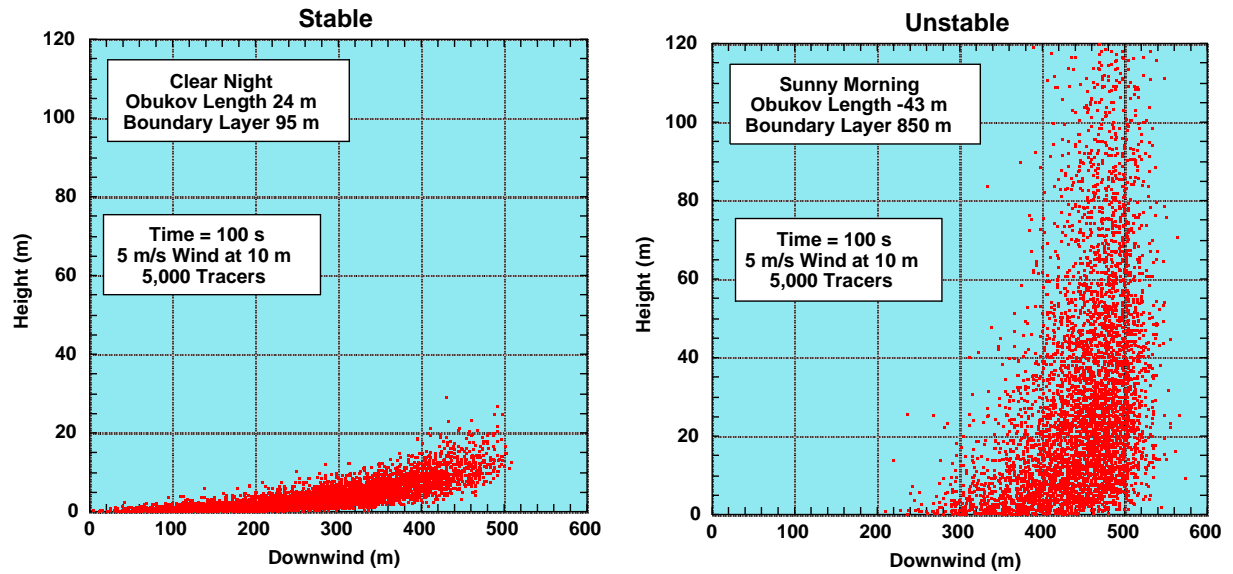


Figure 1. MESO simulations showing tracer locations 100 s after their instantaneous release in both stable (night) and unstable (day) conditions.

of the velocity, both of which have been measured by other investigators as a function of height throughout the BL. (See, for example, Kaimal and Finnegan, 1994). Figure 2 shows a comparison between Hogstrom cloud growth data to that predicted by MESO (solid lines) during stable conditions. By scaling the cloud size by the Eulerian length scale and by scaling the downwind distance by the product of the Eulerian length scale and  $\beta$ , the ratio of the Lagrangian to Eulerian time scales, data from many different stability conditions nearly come together on a single line. MESO predictions are insensitive to the stability when plotted in this manner but do show a distinct difference between the two altitudes at which the data was taken. Hogstrom's data for the high stability conditions (triangles) were also taken at the lower altitude, suggesting that the spread in the data points is related more to altitude than stability. MESO does a good job of predicting the cloud growth except at large downwind distances where the data becomes less reliable.

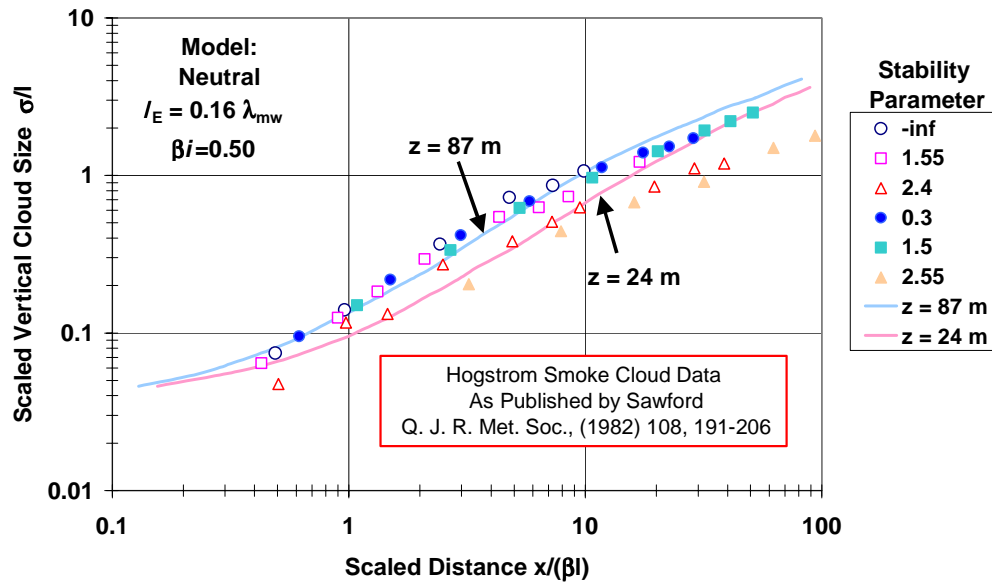


Figure 2. Comparison between the cloud growth data of Hogstrom and that predicted by MESO using the scale-dependent growth theory of Smith and Hay (1961).

Recently, the stochastic tracer technique of Franzese et al. (1999) was installed in the code with an improved equation for the dissipation profile that significantly improved the comparison to test data. The results can be seen in Figure 3 for a continuous release. The two plots show a comparison between the model and the water tank experiments of Willis and Deardorff (1981). Contours of cross-wind integrated concentration are plotted versus both scaled height and scaled time. In the near future, user will be given the option of using either the faster random walk technique or the slower Lagrangian stochastic method.

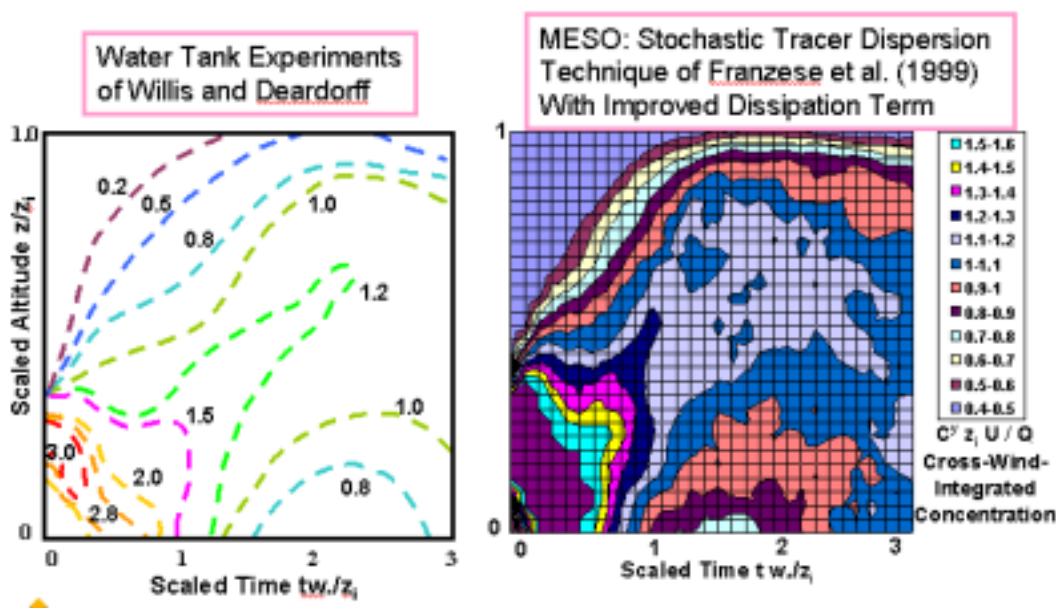


Figure 3. Comparison of the Franzese stochastic tracer technique to the water tank experiments of Willis and Deardorff (1981).

**Heat Flux Modeling** – Since the height of the boundary layer (BL) and the turbulence intensity profile throughout the BL are directly related to the sensible (convective) heat flux, an accurate method of estimating the surface heat budget is key to accurate dispersion modeling. For day or night conditions, MESO contains state-of-the-art heat flux models that require only readily available input parameters such as the relative humidity and surface moisture resistance. Given a vegetation type such as forest or crop variety, standard tables are available for the user to estimate the moisture resistance. Many other models require a Bowen value, which is the ratio between the sensible and latent heat fluxes. For the typical code user, Bowen ratios are usually difficult or even impossible to obtain. Shown in Figure 4 is a plot comparing both measured and predicted values of the four components of the heat budget as a function of time throughout the night from the FIFE data set (Betts and Ball, 1997). Heat radiated away from the ground at night is balanced by the conduction of heat upward in the soil, the convective increase from the warm air, and the gain or loss of heat to evaporation or condensation. In this example, the sensible heat flux starts out with small negative value that corresponds to slightly stable conditions, but then at about 8:00 pm it heads rapidly negative to values that would generate highly stable conditions, followed by a more gentle rise to moderate stability. Although the model shows some error, it follows the trend nicely and is far more accurate than simply giving a constant value throughout the night as often done with most dispersion codes.

**Convective Boundary Layer Model** - To correctly model high-altitude agent releases, a dispersion code must handle the fall and diffusion of the agent down through the convective boundary layer (CBL). As thick as 5 km in desert regions, this layer near the ground is created by wind and solar-generated turbulence (i.e. eddies of warm rising air). The mixing rates in the CBL are usually the highest found in the atmosphere. MESO contains a sophisticated CBL model that predicts both the growth of the CBL and the turbulence characteristics throughout

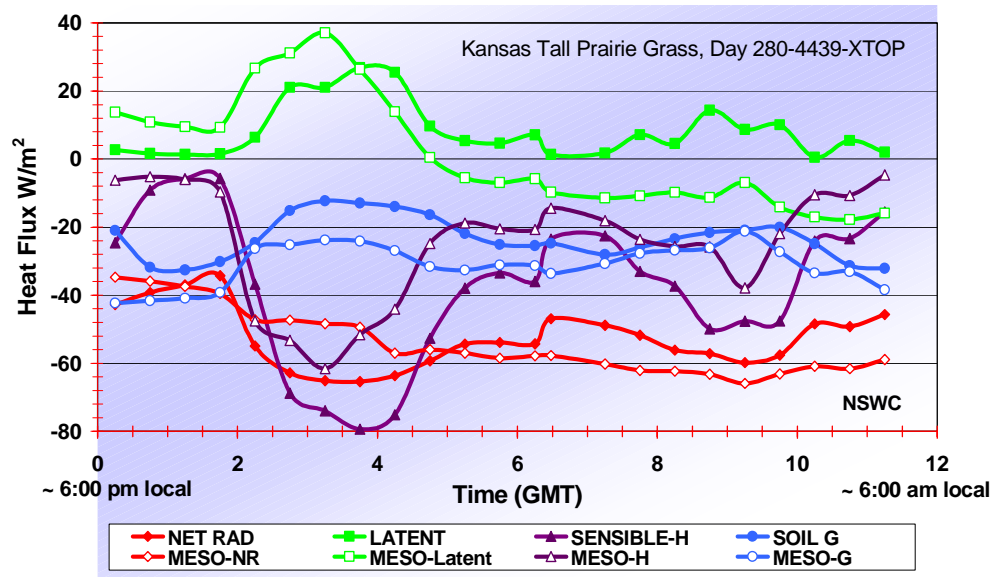


Figure 4. Comparison between measured and predicted heat flux values for the nighttime heat budget.

the CBL. Based on standard surface meteorology and the potential temperature profile, MESO estimates the CBL height by integrating ahead in time a complex rate expression derived by Deardorff (1974). After the CBL height is computed from sunrise, the vertical and horizontal turbulence characteristics can be estimated as a function of height as well. The turbulence parameterization, which is based on numerous measurements found in the literature, is a function of the CBL height and surface meteorology such as the sensible heat flux. As mentioned previously, MESO contains state-of-the-art algorithms to predict the sensible heat flux based on solar flux, cloud cover, wind speed, albedo, humidity, and surface moisture resistance. The predicted growth of the CBL versus time is shown in Figure 5 for a potential temperature profile measured during the summer at the Nevada test site.

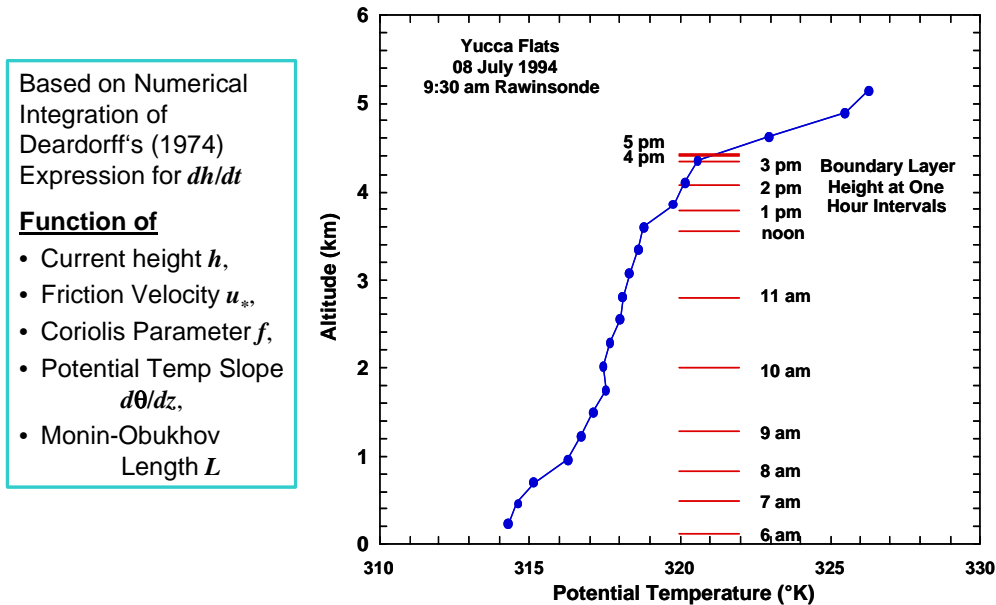
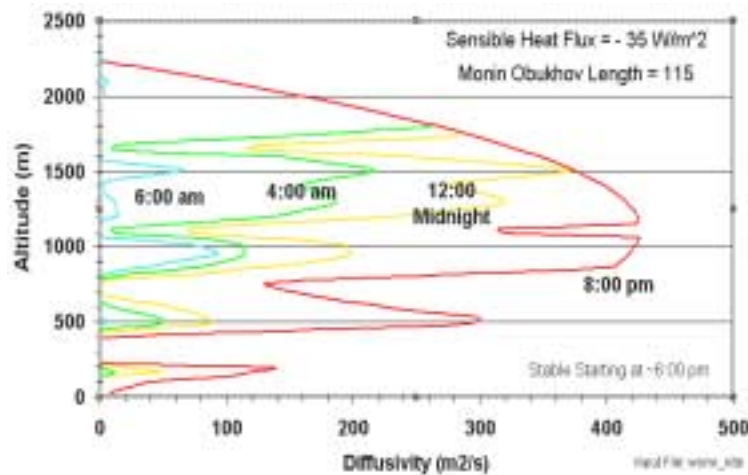


Figure 5. The potential temperature profile is a key ingredient to predicting the growth of the convective boundary layer (CBL), which is indicated by the red lines on an hourly basis. The CBL grows rapidly during midday when solar heating is high, but slows when the temperature slope changes noon.

MESO also models the breakup of the CBL in the early to late evening. Shear instabilities can generate significant turbulence in the layer containing the old CBL long after sunset. Many dispersion codes ignore this fact and erroneously assume highly stable air above the evolving stable boundary layer. To handle this situation, MESO assumes a potential temperature profile based on actual data recorded as a function of time after sunset. Using the sensible heat flux as input, the model applies energy conservation to modify the shape of the profile versus time. Taking into account the wind shear versus altitude, the potential temperature profile is in turn used to estimate a Richardson number needed to compute the diffusivity profile. An example calculation of CBL breakup can be seen in Figure 6, which shows the diffusivity profile at selected times after sunset. As late as midnight, the old CBL layer is well mixed in the top half.



**Figure 6. Breakup of the convective boundary layer versus time.**

A dynamic second-order closure model has also been developed for the boundary layer and is currently being installed in the code. The model is particularly important near or in mountainous regions.

**Clear-Air-Turbulence** - Above the PBL, MESO estimates the vertical eddy diffusivity using both a gravity wave model and a clear-air-turbulence (CAT) model. In low shear regions the diffusion is a function the potential temperature slope and the turbulent velocity variance, which in turn is estimated from gravity wave predictions. In high shear layers the model employs a CAT algorithm based on the amount of shear found across the layer. In the U.S. Army's Crystal Mist high-altitude test series, model predictions of high CAT diffusion correlated well with the observed rapid growth in the measured cloud size, thus confirming the use of CAT techniques within MESO. When not in CAT layers, the measured clouds grew quite slowly in the vertical direction, consistent with low values of vertical diffusivity predicted by the gravity-wave model in MESO. A comparison between MESO and the Crystal Mist lidar data is shown in Figure 7 for a cloud of small glass beads released at an altitude of nearly 7 km. The data was recorded nearly an hour after the cloud release. In the upper atmosphere, true horizontal diffusion is quite low. In the Crystal Mist test series, the horizontal spread in the clouds was found primarily to be due to the interaction of vertical mixing with vertical shear rather than due to horizontal turbulent mixing.

**Deposition Modeling** - MESO accurately computes the turbulent deposition of particles at the ground--a feature important for the long-range transport of small particles such as agents of biologic origin. When the deposition rates are high, such as for small particles over vegetated terrain, the deposition can significantly deplete the base of an agent cloud, resulting in exposures further down wind that are as much as a factor of three lower than predicted by a typical Gaussian puff dispersion code. Using tracer particle techniques the deposition at the ground can be computed by MESO to a high degree of accuracy. MESO contains a high-fidelity algorithm to estimate the deposition rate based on particle size and density, wind speed, stability, surface roughness and surface resistance. The algorithm accurately predicts deposition due to turbulence over a rough surface, as well as deposition due to vegetation filtration. Figure 8 shows a comparison between the model predictions and actual data as a function of particle size for a grass surface.

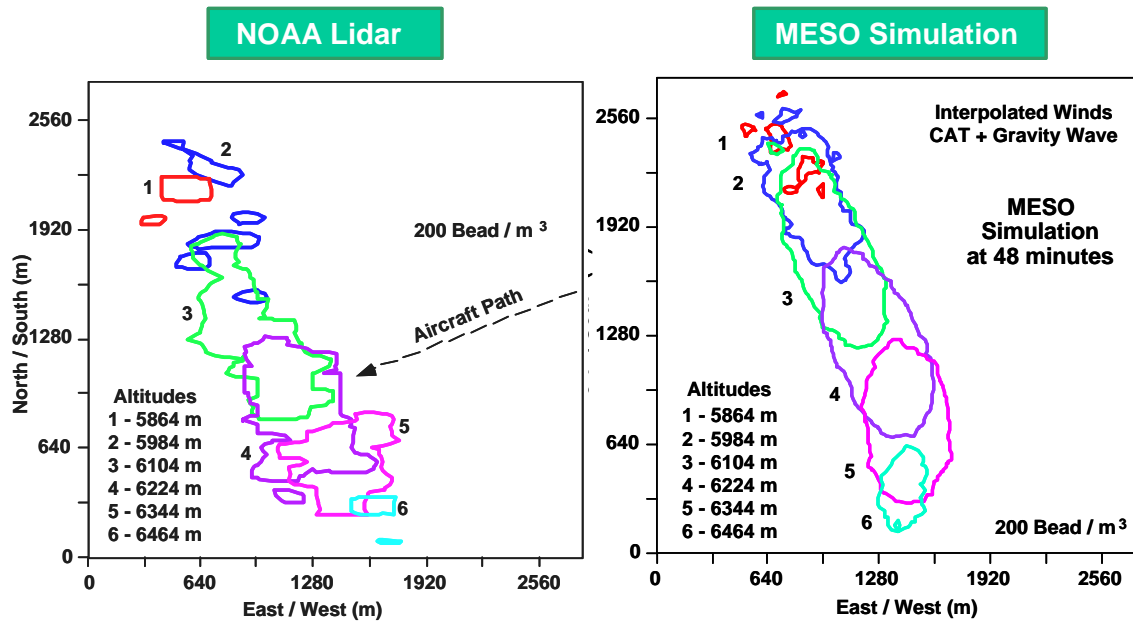


Figure 7. Comparison between high-altitude lidar data and a MESO code prediction at 48 min after release for a case involving a strong clear-air-turbulence layer.

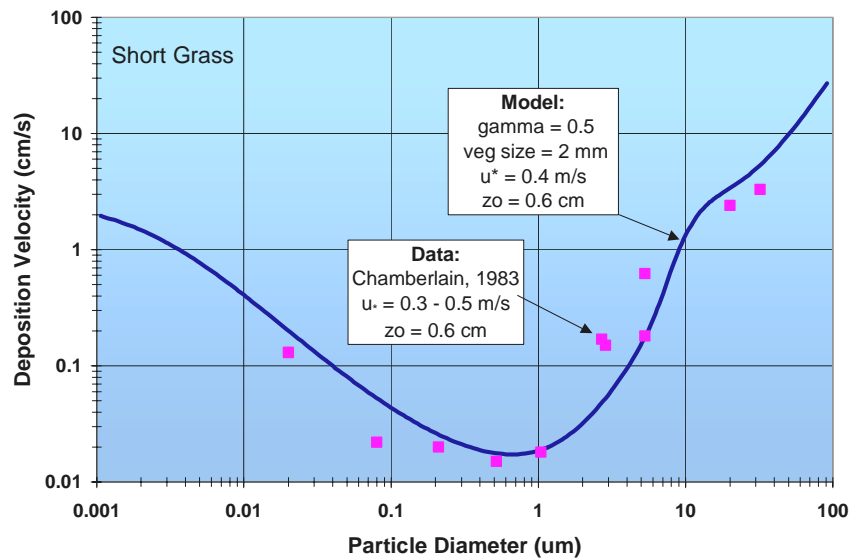


Figure 8. Comparison between the predicted and measured rate of deposition versus particle size over a grass surface in light winds.

**Dose/Deposition Variance** – Because of the highly chaotic nature of atmospheric turbulence, a cloud of agent released in the atmosphere may travel in a nearly random direction that is as much as 90 degrees from the mean wind direction. Furthermore, updrafts or downdrafts due to heat rising from the ground can result in the lofting of a cloud, or worse, a rapid sinking of the cloud that presents high concentrations to people nearby. Predictions of dose and deposition variance are necessary ingredients in the estimation of downwind casualties following the release of chemical or biological agents. New algorithms have recently been installed in MESO to estimate



dose/deposition variance and probability of occurrence. The goals of this effort were quite ambitious. The algorithms must accurately handle:

- Flow through complex terrain
- Droplet size distributions for liquid chemical releases
- Evaporating chemical droplets that settle rapidly
- Simultaneous dispersion and transport of droplets and vapor
- High deposition rates (such as with biological agents in highly vegetated regions)
- Both stable and unstable conditions
- Both horizontal and vertical turbulence throughout the boundary layer

The technique involves tracking four tracer clusters. One cluster consists of plume tracers that are converted to cloud path tracers (Luhar et al., 2000). The other three clusters are handled as clouds with scale-dependent dispersion. Each of these three is forced to follow a vertical path based on the path tracer distribution, but the horizontal path is directly downwind. Dose and deposition files are saved for these three clouds every code advection cycle. Then, at the end of the run the clouds are moved over many different horizontal paths based on the cloud path statistics that were also saved each cycle. Statistics are recorded for each of the many cloud paths to permit the calculation of conditional probability, i.e. the probability that the dose will exceed a given dose or deposition will exceed a given deposition. Contour plots of conditional probability for vapor dose are shown in Figure 9 for the release of 100 kg of GB agent droplets at an altitude of 100 m with the CBL height at 470 m. Although only a small region near the release exceeds an average dose of  $1 \text{ mg-min/m}^3$ , the probability of exceeding this value is finite over a much wider region.

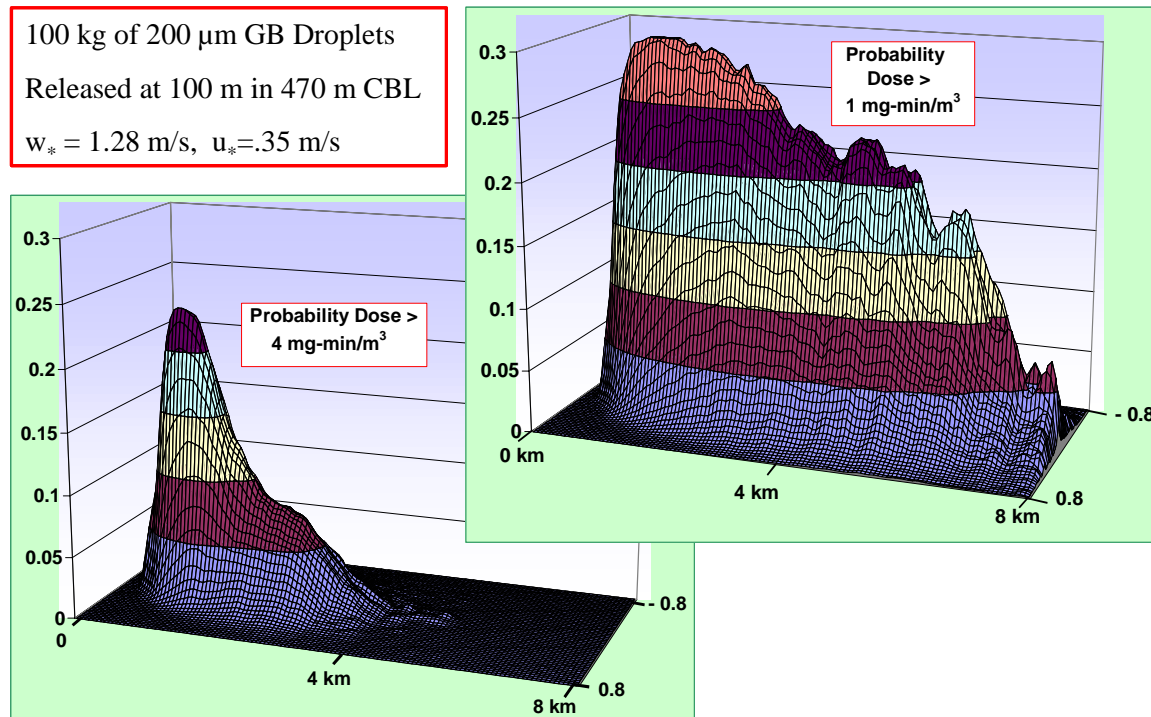
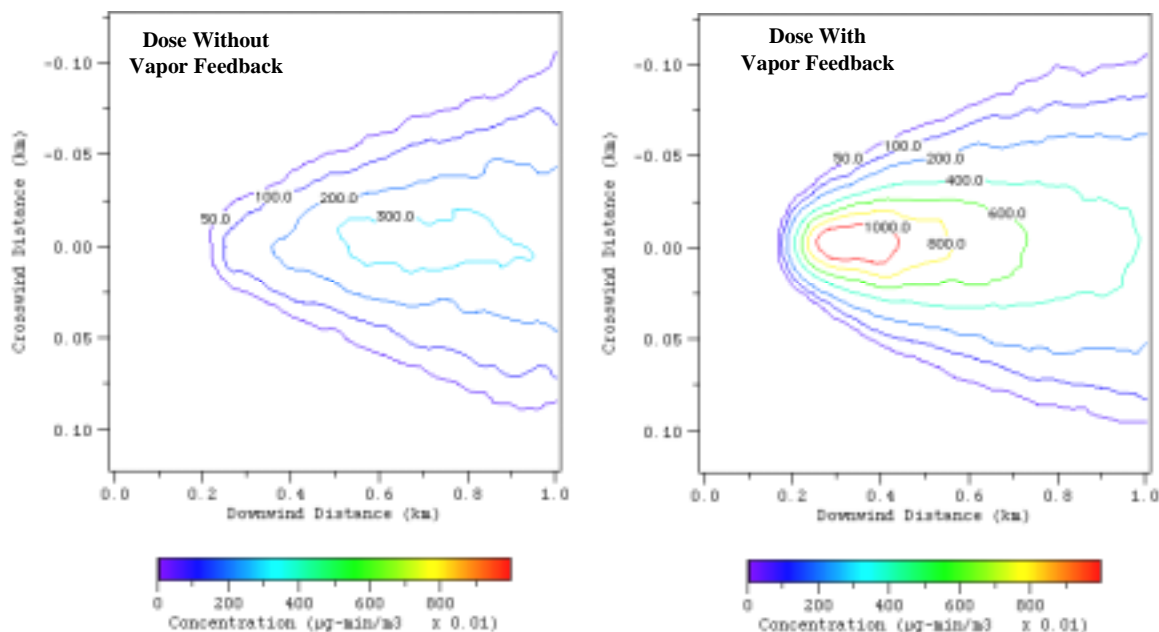


Figure 9. Probability that a dose of  $4 \text{ mg-min/m}^3$  (left) and  $1 \text{ mg-min/m}^3$  (right) is exceeded for vapor generated by the evaporation of 100 kg of GB droplets released at a height of 100 m.

**Source Options** - In a typical MESO application, the agent source is defined as a normally distributed group of particles with the vertical and horizontal variance input by the user. However, for the investigation of leaking (damaged) TMD threat missiles, a line source option is available. The source can be an instantaneous release, a

continuous release (plume), or a timed release. For either chemical or biological agents, the user can select a lognormal size distribution. MESO contains routines to estimate the gravitational fall velocity of droplets for particle sizes from microns up to a few millimeters, thus covering the range from bio particles to large chemical droplets. Diffusion rates are reduced with increasing droplet size to account for inertial effects. For chemical droplets, MESO uses a state-of-the-art numerical evaporation routine that includes vapor feedback to limit the evaporation rate. As droplets evaporate, vapor tracers are spawned in the vicinity of the evaporating droplets. Routines to handle secondary evaporation due to droplets that have deposited on the ground are included. Figure 10 shows predicted dose contours both with and without vapor feedback following the release of 100 kg of GB droplets at a height of 50 m. Without vapor feedback to limit the evaporation rate, the droplets evaporate at higher altitudes resulting in significantly less dose near the release point.



**Figure 10. Predicted ground-level dose from vapor following the release of 100 kg of GB 100 µm droplets at a height of 50 m. Without vapor feedback to limit the evaporation rate, the droplets evaporate at higher altitudes resulting in significantly less dose near the release point.**

**Output Options** - A full compliment of routines have been installed in MESO to generate output grids of concentration, deposition, or time-integrated concentration (dose) at any altitude of interest. Recently, grids containing conditional probability were added to the list of out types.

**Validation** – As shown above, many of the submodels in MESO have been carefully validated. Direct validation against dispersion data is currently underway at NSWC. MESO predictions compare well against measurements of high-stack emissions, ground level lidar data, short-range concentration data, as well as against high-altitude (Crystal Mist) lidar data.

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